

Abstract

Hydroxychalcone Color Indicators for pH and Fluoride Ion [†]

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Abstract: Chalcone composed of two aromatic rings bridged by an α,β -unsaturated carbonyl group, exhibits a variety of biological activities. With an objective to develop a novel chalcone-based functional dye, we have synthesized a chalcone diol, bearing two OH groups at the 2-positions on both phenyl rings, and found that it serves as color indicators for pH and fluoride ion.[1] The chalcone diol showed a vivid color change from colorless to yellow (halochromism) in water at pH ≥ 10 . Further, it also showed a selective color change from colorless to red through chemical sensing of fluoride ion in CH₃CN. The absorption spectral study together with TD-DFT calculations and X-ray crystallographic analysis revealed that the characteristic π -resonant structures of the chalcone diol caused by OH-F⁻ interactions and the planar conformation owing to its intramolecular hydrogen bonding may provide a strong charge transfer (CT) absorption in the visible region.

The observed results and the mechanisms revealed in this study provide important ideas and strategies for the future molecular design of chalcone-based chemosensors and bioactive substances.

Keywords: chalcone; fluoride ion; TD-DFT

Reference

1. Du, Y.; Liang, F.; Hu, M.; Bu, R.; Wang, M.; Tsuda, A.; Eerdun, C. Hydroxychalcone dyes that serve as color indicators for pH and fluoride ions. *RSC Advances* **2020**, *10*, 37463–37472.